

RELEASE\_NOTES 12 September 2003

The major changes and new features of this release are:

- 1) Modified the treatment of secondary organic aerosol (SOA) formation
  - + The SOA algorithm has been modified to make the gas-particle partitioning of semi-volatiles reversible
  - + Eliminated SOA production from anthropogenic alkenes
  - + Adjusted yields of semi-volatiles from alkanes and aromatics to account for emissions of non-SOA producers being lumped with those from SOA-producers
  - + Modified gas-phase monoterpene reactions rates in RADM2 and CB4
- 2) Modified the heterogeneous N2O5 reaction probability
- 3) Added an Euler Backward Iterative (EBI) gas-phase chemistry solver for the CB4 family of chemical mechanism
- 4) Implemented layer-dependent horizontal advection time-stepping
- 5) Changed the order of the time splitting science processes:

Previous order	New order
advection	vertical diffusion
mass-adjustment	advection
horizontal diffusion	mass-adjustment
vertical diffusion	horizontal diffusion
clouds	clouds
chemistry	chemistry
aerosols	aerosols
- 6) Updated all gas-phase chemical mechanisms (cb4, radm2, saprc)
  - + New deposition velocity surrogates
  - + New cloud scavenging surrogates
  - + Zeroed reaction rate constant for  $\text{N}_2\text{O}_5 + \text{H}_2\text{O} \rightarrow 2\text{HNO}_3$  in all /aero3 mechanisms
  - + Changed names of aero3/SOA NR species
  - + For CB4, eliminated advection and diffusion of fast-reacting species
- 7) Cloud enhancements/updates
  - + Modified to use effective Henry's Law constant for scavenging
  - + Updated and added new coefficients to the Henry's Law constant table
  - + Revised the timestep calculation in the aqueous chemistry subroutine
  - + Updated the coarse-mode aerosol number washout

- 8) Other enhancements and bug fixes
- + Changed the units for aerosol for vertical diffusion to molar mixing ratio instead of mass density concentration
  - + Updated the minimum aerosol concentration array and bug fix in coarse-mode aerosol standard deviation in the aerosol dry deposition subroutine
  - + Added compatibility with emissions files that contain PM10 and speciated PM2.5 but do not contain PMC
  - + Removed unused SUBST\_GRID\_ID
  - + Fixed index bug in load\_cgrid
  - + Bug fix for no gas emissions species
  - + Fixed NFS latency problems for parallel runs on an MPICH cluster
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RELEASE\_NOTES 8 May 2003

The major changes and new features of this release are:

- 1) Scripts to build and run CMAQ for MPICH Linux clusters
  - 2) Incorporation of the I/O API Version 2.2
  - 3) Some enhancements and bug fixes:
    - + Modifications of the vertical diffusion module were made to improve data locality to speed up computation.
    - + A bug was fixed for the case where a user would build a model for no aerosols.
    - + Changes were made to improve robustness for inexact I/O API (netCDF) file header data.
    - + Some codes were modified to correct Fortran compiler errors with some vendors.
    - + For the heterogeneous N2O5 reaction in the aerosol module, an error was corrected in the concentration units for calculating the HNO3 yield. Also, the rate constant calculation for this reaction has been changed to use effective radius instead of diameter.
    - + An error in the contribution of N2O5 to total initial HNO3 has been corrected in the cloud module. Also, the MAX function was changed to MIN to correct a bug in the calculation of TOTFRAC.
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RELEASE\_NOTES 9 July 2002

The major changes and new features of this release are:

- 1) A new aerosols module, `aero3`, that includes:
  - + improved treatment for Secondary Organic Aerosol formation by including semivolatile compounds that partition between gas and aerosol phases,
  - + updated process for Sulfate nucleation,
  - + heterogeneous conversion of  $\text{N}_2\text{O}_5$  to Nitric Acid,
  - + incorporate the ISORROPIA model for thermodynamics.
- 2) Incorporate aerosol emissions in the vertical diffusion process.
- 3) Change the order of the time splitting science processes:
  - from chemistry -> clouds -> aerosols
  - to clouds -> chemistry -> aerosolsto provide a better linkage between gas-phase chemistry and aerosols.
- 4) Add the Sapr99 gas-phase mechanism and all CMAQ variants.
- 5) Add Modified Euler Backward Iterative (MEBI) solvers for all variants of CB4, SAPRC99, and the RADM2-Carter-4-Product-Isoprene mechanisms.
- 6) Add a new vertical diffusion module, the Asymmetric Convective Model (ACM).
- 7) Change to a dynamic allocation of the horizontal grid for the chemistry model (CCTM) and the initial and boundary concentrations pre-processors (ICON and BCON). This allows one executable to run any horizontal domain that CMAQ supports.
- 8) In conjunction with (7), CCTM now can window from meteorology and emissions datasets, so that runs on many subdomains can be executed using one dataset that encompasses all those subdomains.
- 9) Addition of hour-averaging output option for any chemical species.